STUDIA UNIVERSITATIS BABEŞ-BOLYAI, CHEMIA, LI, 1, 2006

MODELLING URANIUM(VI) EXTRACTION USING ARTIFICIAL NEURAL NETWORKS

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Dedicated to professor Sorin Mager
at his 75th anniversary

ABSTRACT. The use of ANN simulators for the mathematical modelling of the uranium(VI) extraction from an aqueous solution, using polar and/or nonpolar solvent containing the chelating agent di-(2-ethylhexyl)-ditiophosphoric acid, at different pH values is described. The ANN has been trained with experimental data using either 1-butanol or kerosene solvent. Good prediction results show the incentives of this modelling approach and the perspectives of its using for simulating processes with the aim of optimising both laboratory and industrial units.

Introduction

Artificial Neural Networks (ANNs) are founded on an idealized representation of the biological cell that processes information. ANNs can be represented as weighted directed graphs consisting in simple elements, neurons (grouped in layers) operating in parallel, and the connections between neurons. The weighted connection paths link every two neurons from adjacent layers such as the weighting structure is able to provide the overall network performance. As the ability to learn is a fundamental trait of intelligence, the ANNs may be considered simple but powerful artificial intelligence elements. In the ANNs context the learning process consists in updating the network architecture and connection weights so that the network can efficiently achieve a specific task. Usually, the tasks an ANN may effectively perform are: pattern classification, clustering or categorization, function approximation, prediction and associative memory applications [1].

But the main benefits of the ANN approach consist in their remarkable ability for generalization. The use of ANN models for control purposes has gained considerable attention in the field of modelling chemical process, being the subject of several scientific reports, and they are increasingly applied for system identification and simulation [2]. As a consequence, the ANNs may be successfully used for modelling systems in which detailed

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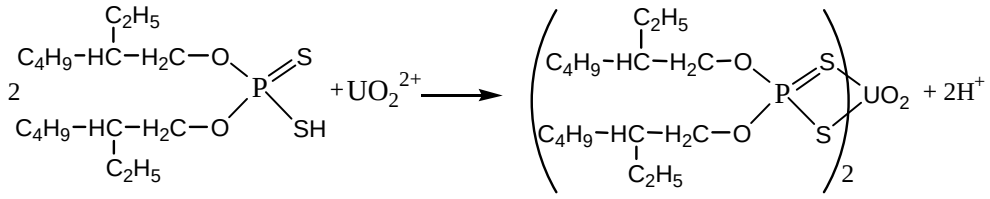
governing rules are unknown or difficult to formalize under the form of first principle models [3, 4]. This last capability is exactly the type of application the present work is aimed to achieve.

The extraction of uranium(VI) from aqueous solutions with immiscible polar or nonpolar solvents using a dithiochelating agent was extensively studied. The choice of the proper solvent [5, 6] as well as the choise of the ligand [7, 8] and the optimal pH range were previously investigated.

This paper presents a first attempt to use Artificial Neural Networks for predicting the extraction of uranium(VI) from an aqueous solution, using mixtures of polar/nonpolar solvent of different ratio, in the presence of the chelating ligand di-(2-ethylhexyl)-ditiophosphoric acid. The chelate formation reaction is presented in scheme 1.



Scheme 1

Results and Discussions

The Artificial Neural Network employed in this study is of feedforward type and the backpropagation algorithm has been used for training the network's biases and weights. The network configuration is of multilayer structure and the quasi Newton Levenberg-Marquardt backpropagation algorithm has been used for learning.

The ANN architecture has been designed on the basis of heuristic methods. Its structure consists in an input layer of three neurons, a hidden layer of four neurons and a single-neuron output layer. The activation function of the first and second layer is of *tansig* (tan-sigmoid) form but the activation function of the output neuron is *linear*.

First, the ANN has been trained using the following input-output (input-target) pairs of data:

- ***Inputs*:** experimental data for the extraction of uranium(VI) from an aqueous solution having the uranium(VI) concentration of 0.1212 g/l, with either 1-butanol or kerosene solvent containing the chelatization ligand di-(2-ethylhexyl)-ditiophosphoric acid, at different pH values; these experimental data are presented in Table 1.

- ***Outputs*:** experimental data consisting in the percentage values of uranium(VI) extraction obtained for the above mentioned inputs, also presented in Table 1.

Table 1.

Experimental data for the extraction of uranium(VI) from an aqueous solution ($C_{U(VI)}$=0.1212 g/l), with either 1-butanol or kerosene solvent containing the chelatization ligand di-(2-ethylhexyl)-ditiophosphoric acid, at different pH values.

Sample no.	1-Butanol solvent		Kerosene solvent	
	Intputs pH	Outputs E [%]	Intputs pH	Outputs E [%]
1	1.2	94.5		
2	2.0	96.4		
3	4.1	99.2		
4	4.7	99.8		
5	5.6	99.9		
6			1.05	13.4
7			1.21	21.4
8			2.0	55.4
9			2.8	85.9
10			4.1	87.8
11			4.7	87.2
12			5.6	85.8

The ANN has been successfully trained. The simulation results produced by the trained network for modelling the percentage values of uranium(VI) extraction confirm this statement. The results (outputs) obtained by simulation for the already trained ANN, having as inputs the data presented in Table 1, are compared to the experimental outputs presented in the same table. The comparative results between experimental and ANN simulated data are shown in figure 1.

The relative errors between the ANN simulated data and the experimental data are considered to be small, as their offset is limited to ±1.4 %.

Second, as one of the most appreciated properties of the ANNs is their ability to make predictions, this was also the main purpose of the presented investigation. The predictions consist of the ANN's aptitude to provide values of the outputs for the inputs not yet seen during the training step.

During this second testing step the already trained ANN has been used for predicting the values for the percentage extraction of uranium(VI) from the aqueous solution ($C_{U(VI)}$=0.1212 g/l) containing 1-butanol *and* kerosene solvents with concentrations of various ratios, having totally different values compared to the ones used during the training step.

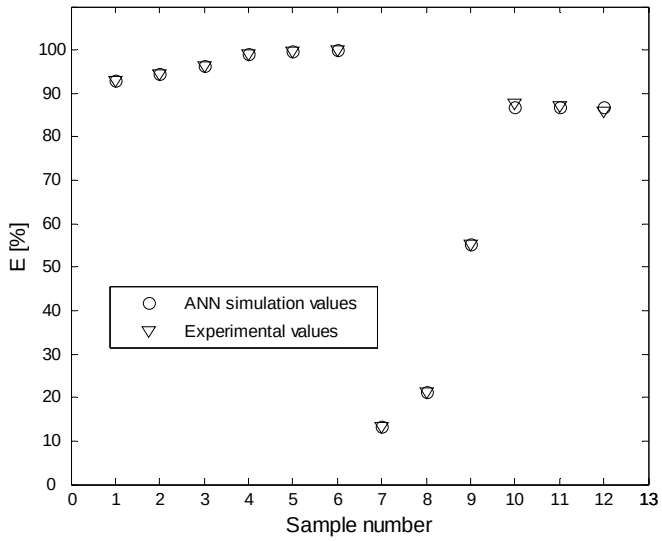


Fig. 1.
Comparative results between ANN simulated data and experimental data, for the set of input-output data used for training the ANN (*learning*)

In order to test the prediction capability of the trained ANN a new set of input-output experimental data has been used, as they are presented in Table 2.

Table 2.
Experimental data for the extraction of uranium(VI) from an aqueous solution ($C_{U(VI)}$=0.1212 g/l), using various 1-butanol-kerosene solvent mixtures containing the chelating ligand di-(2-ethylhexyl)-ditiophosphoric acid, at the pH values 2.5-3

Sample no.	$C_{butanol}$ [% vol. in kerosene]	E [%]
1	5	97.00
2	10	99.84
3	20	99.60
4	30	99.76

The values for the percentage extraction of the uranium(VI) obtained by ANN simulation are compared with the experimental values shown in Table 2 and the comparative results are presented in figure 2.

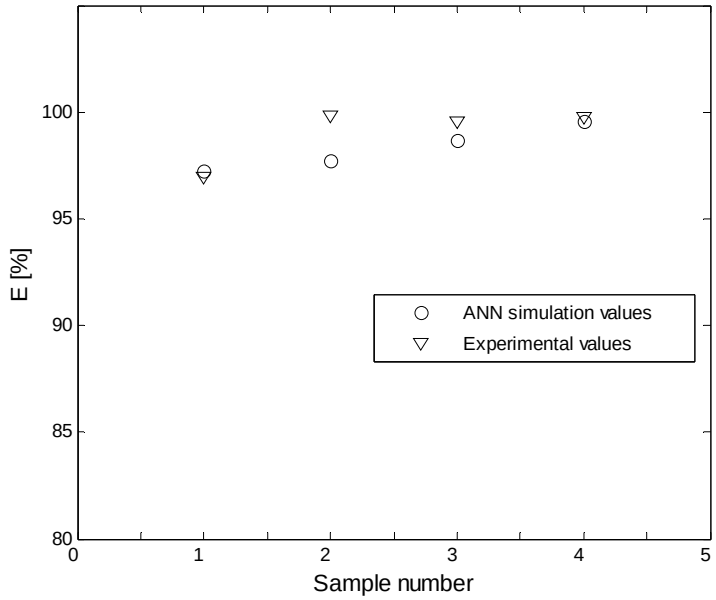


Figure 2.
Comparative results between ANN simulated data and experimental data, for the set of input-output data used for ANN testing (*prediction*).

As it may be noticed from figure 2, the ANN has good predictions capabilities proved by the errors situated in a narrow interval of ± 2.5%. Additionally it may be mentioned that testing has been performed on an input-output set of data not encountered during the ANN training procedure, and with the inputs having values very different to those used for training.

Conclusions

Although a relatively limited set of data has been used for training the results obtained on the basis of an ANN model for the simulation of the extraction of uranium(VI) from an aqueous solution ($C_{U(VI)}$=0.1212 g/l), using various 1-butanol-kerosene solvent mixtures containing the chelating ligand di-(2-ethylhexyl)-ditiophosphoric acid are very promising, The simulator may be used for getting new sets of data for uranium(VI) extraction using 1-butanol-kerosene solvent mixtures, sparing experimental time and costs. Further improvement of the model may be performed by the use of a more extended training set of data.

The use of ANN simulators for the mathematical modelling of the uranium(VI) extraction from an aqueous solution with 1-butanol - kerosene solvent mixtures containing the chelating ligand di-(2-ethylhexyl)-ditiophosphoric

acid may become a very useful tool for both laboratory and industrial scale optimisation of this investigated process.

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